3rd International Conference on

# Smart Materials & Structures

March 20-22, 2017 Orlando, USA

# Scientific Tracks & Abstracts

## Day I

Patrice Woisel, J Material Sci Eng 2017, 6:2 (Suppl)
http://dx.doi.org/10.4172/2169-0022.C1.061

# Supramolecular chemistry: A powerful tool to elaborate colorful multi-stimuli responsive macromolecular materials

**Patrice Woisel**
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There is no doubt that the creation of high performance polymeric materials relies directly on our ability to manipulate these smart materials in a controllable, predictable and orchestrated fashion from nano to macro-scale. Recently, architectures where the individual polymer blocks are connected through supramolecular interactions such as hydrogen bonding, metal-ligand and pseudorotaxane like interactions have received significant attention. The inherent features of the molecular recognition-driven self-assembly confer significant advantages over their covalently linked brethren in terms of facilitating modularity and self-healing properties. Moreover, through careful design smart polymeric systems have been developed with stimuli-responsive structures and properties. Here, we report the successful engineering of new multi-stimuli responsive and colored macromolecular assemblies based on well-defined functionalized polymer building blocks incorporating both electro-deficient ($CBPQT^{4+}$) and electron-rich units (tetrathiafulvalene, naphthalene) moieties. The architectures of these materials have been constructed by specifically holding together complementary well-defined polymer building blocks (prepared by Controlled Radical Polymerization) with specially designed host/guest motifs attached in specific locations on polymer backbones. The inherent reversibility of supramolecular architectures has allowed on demand modular and tunable modification of structures and properties of materials. More particularly, we have exploited the presence of colored $CBPQT^{4+}$ based interactions to create smart micelles and hydrogels and reprogrammable supramolecular temperature and pH sensors with memory function. An important practical aspect of these new functional materials is that all relevant phenomena (self-assembly and disassembly processes, reading/reprogramming of temperature, memory function) have an associated visible readout, thereby affording convenient and quantifiable systems with applications spanning the physical and biological sciences.

## Biography

Patrice Woisel has obtained his PhD in Organic Chemistry at the University of Lille, France in 1996 and was appointed as a Lecturer at the University of Dunkerque, France. In 2007, he became a Professor at the National School of Engineering Chemistry (ENSCL), France. He currently leads a research group of around 10 people and has written over 90 publications in major international journals.

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**Notes:**

Dong Joo Kim et al., J Material Sci Eng 2017, 6:2 (Suppl)
http://dx.doi.org/10.4172/2169-0022.C1.061

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3rd International Conference on

Smart Materials & Structures

March 20-22, 2017 Orlando, USA

# The damage self-sensing response of ultra-high-performance fiber-reinforced concrete in tension

**Dong Joo Kim** and **Min Kyoung Kim**
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In this study, the change of electrical resistivity in Ultra-High-Performance Fiber-Reinforced Concrete (UHPFRCs) in tension was investigated. UHPFRCs have shown significant reduction in their electrical resistivity after first cracking until post cracking tensile strength point during their unique tensile strain-hardening. An experimental program was designed to investigate the change in the electrical resistivity of UHPFRCs blending 1 vol.% long (L=30 mm, D=0.3 mm) and 1 vol.% short (L=19 mm, D=0.2 mm) smooth steel fibers. To measure the electrical resistivity, a layer of silver paste was first applied onto the surface of specimens and then copper tapes were attached on the silver paste. The distance between two outsides electrodes for input current (10 μA) was 110 mm while that between two electrodes for voltage measurement was 50 mm. The specimen was subjected to direct tension using a universal testing machine (UTM). The speed of the machine displacement was 1.0 mm/min. The reduction in the electrical resistivity of UHP-FRCs under direct tension until post cracking tensile strength was 437.7 kΩ·cm, and it was found to be significantly higher than those (13.7 and 149.7 kΩ·cm) of strain hardening steel-fiber reinforced concretes (SH-SFRCs) with lower strength matrices (117 and 152 MPa), respectively. The potential damage-sensing capacity of UHPFRCs, in addition to the high mechanical resistance of UHPFRCs, would be considerably favorable for future structural health monitoring system as well.

## Biography

Dong Joo Kim has his expertise in the development and evaluation of high performance cement based construction materials with high tensile strength, ductility and energy absorption capacity in addition to self-sensing or self-healing capability. He has obtained his PhD degree from the University of Michigan, Ann Arbor in 2009 and since then he has been an Assistant and Associate Professor in Sejong University, South Korea.

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**Notes:**

Liying Jiang et al., J Material Sci Eng 2017, 6:2 (Suppl)
http://dx.doi.org/10.4172/2169-0022.C1.061

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Smart Materials & Structures

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# Investigation on electromechanical harvesting schemes to improve the performance of viscoelastic dielectric elastomer generators

**Liying Jiang, Jianyou Zhou** and **Roger Khayat**
University of Western Ontario, Canada

As a category of electroactive polymers, dielectric elastomers (DEs) exhibit physical response to electrical stimuli and transduce electrical energy to mechanical energy. On the other hand, when acting in a generator mode, they can also convert mechanical energy from different sources, such as winds, ocean waves and human movement into electrical energy. Due to their flexibility and high energy density, dielectric elastomer generators (DEGs) have recently attracted much attention from the research community. It has been demonstrated in experiments that DEGs can achieve energy densities more than 10 times higher than those of piezoelectric and electromagnetic generators. Although some DEGs have shown very promising results, their performance is in fact affected by multiple failure modes and the material viscoelasticity. Particularly, the material viscoelasticity of the DE membrane embedded in a DEG could cause high energy dissipation of the generator and exert a strong influence on the design of its harvesting scheme. To uncover possible approaches to improve the performance of DEGs, this work presents a framework to comprehensively evaluate the harvested energy and conversion efficiency of DEGs with the consideration of the finite-deformation viscoelasticity of the material. Also, different possible energy harvesting schemes are explored in this work. From our simulation results, it is found that choosing a suitable voltage level of the power supply (or a suitable bias voltage) could markedly raise both the harvested energy and conversion efficiency of DEGs. The general framework and results in this work are expected to provide insight into optimizing the design of dielectric elastomer generators.

## Biography

Liying Jiang is an Associate Professor at the Department of Mechanical and Materials Engineering, University of Western Ontario, Canada. She has received her PhD from the University of Alberta in 2005. Her research interests and activities cover a wide range of applied mechanics. Her expertise is theoretical and numerical simulation to develop mechanics and physics models for challenging problems related to material's behavior ranging from traditional composites to smart materials and to nanostructured materials.

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## Notes:

Elias Torres Alonso et al., J Material Sci Eng 2017, 6:2 (Suppl)
http://dx.doi.org/10.4172/2169-0022.C1.061

## Wearable electronics based on graphene-coated conductive textile fibers

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[2]University of Aveiro, Portugal

The concept of smart-textiles is witnessing a rapid development with recent advances in nanotechnology and materials engineering. Bearing in mind that the concept of textiles is much wider than clothes and garments, the potential is immense. While most current commercial applications rely on conventional hardware simply mounted onto fibers or fabrics, a new approach to e-textiles consisting in using functionalized textiles for several technological applications has the potential to change the paradigm of wearable electronics completely. Conducting fibers are an important component of any e-textile, not only because they can be used as wiring for simple textile-based electronic component, but also because they can be used to build electronic devices directly on textile fibers. We have reported a new method to coat insulating textile fibers with monolayer graphene to make them conductive while preserving their appearance. There are a number of factors that can greatly influence the sheet resistance achieved by graphene-coated textile fibers. In order to understand the influence of the topography of the fibers on the effectiveness of the graphene coating, an extensive study encompassing microscopy techniques like Atomic Force Microscopy and Scanning Thermal Microscopy, as well as Raman spectroscopy was performed. This method has proven to be a versatile tool to achieve flexible, transparent and conducting fibers of different materials, sizes and shapes. The first applications of electronic devices built on such fibers are demonstrated with an alternating current electroluminescent device, following previous work in our group on similar devices in flexible substrates. This opens up the way for the realization of wearable devices on textiles.

### Biography

Elias Torres Alonso has a background in Physics with a specialization in Physics of Materials in the Complutense University in Madrid. After that, he obtained an Erasmus fellowship to spend one year in Lund University in Sweden, where he worked with III-V Nanowires. At the moment, Elias is working towards his PhD in Physics/Engineering at the University of Exeter, United Kingdom, where he uses various 2D materials to create flexible, wearable and scalable next-generation electronic and optoelectronic devices within the group of Prof Monica Craciun and Prof Saverio Russo.

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**Notes:**

Nusrat Jahan et al., J Material Sci Eng 2017, 6:2 (Suppl)
http://dx.doi.org/10.4172/2169-0022.C1.061

# Development of piezoelectric properties in PVDF: Effect of particle concentration and stretching variables

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Polyvinylidene fluoride (PVDF) has relatively high thermal stability (~120 °C) with moderate piezoelectric coefficient ($d_{33}$~30pC/N) while cellular polymers such as polypropylene (PP) has higher $d_{33}$ value (120-600 pC/N) with poor thermal stability (up to around 50 °C) which limited their applications in high temperature transduction. Therefore, a three-phase composite has been studied where organoclay has been added to enhance polar β phase and $CaCO_3$ to introduce cellular structure in PVDF to get the advantage from both source of piezoelectricity with thermal stability. The samples were prepared by mixing PVDF, organically modified nanoclay (1-12 wt%) and $CaCO_3$ (30-40 wt%) into a twin screw extruder and subsequent calendaring of films with thickness around 100 µm. FTIR result showed that although the supplied $CaCO_3$ is not surface modified, still it results in around 30% of β phase in PVDF in absence of nanoclay and a gradual increase was observed in β phase with increasing amount of $CaCO_3$ and this increment was further elevated by adding surface modified organoclay. Though various percentage of clay was used, 3 wt% of them seems to contribute maximum β phase (~55%) due to better dispersion and DSC as well as XRD confirmed the results further. Maximum 87% β phase was found in PVDF/40 wt% $CaCO_3$/3 wt% nanoclay sample after stretching at a ratio (R=final length/initial length) of 4.5 at 90 °C. Seemingly, increased stretching ratio not only improved the β phase content but also created harmonious voided structure around $CaCO_3$ particles in the sample. SEM on stretched film showed the presence of such lenses shaped voided structure inside the film.

## Biography

Nusrat Jahan has completed her MSc from Tuskegee University, USA and currently pursuing PhD in Ecole Polytechnique de Montreal, Canada. She has published 5 papers in journals and in a couple of proceedings.

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**Notes:**

Ihsan Burak Temelturk et al., J Material Sci Eng 2017, 6:2 (Suppl)
http://dx.doi.org/10.4172/2169-0022.C1.061

# Design optimization, control and experimental characterization of flapper mechanism with amplified piezo actuator

**Ihsan Burak Temelturk** and **Melin Sahin**
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Servovalves are critical sub components of hydraulic systems which are used in many fields such as aerospace and defense technologies. Conventional servovalves have torque motor which has a shortcoming of narrow bandwidth and long response time which result in a bulky behavior of the overall system. Usage piezoelectric actuator is a novel way to overcome this problem. In this study, design of a first stage flapper of a two stage servovalve involving a mechanically amplified piezo-stack actuator instead of a torque motor is done. In the design problem, flapper displacement and the force developed at the nozzle location are set as the design objectives. Thickness and the height of the flexure are the design variables regarding the flexure. Finite element method and mathematical modeling of piezo actuators and structures are utilized to build a model of the first stage of the servovalve with piezoelectric actuator. Design parameters of amplification mechanism of piezo actuator are verified by finite element analyses and experimental results. Dynamic behavior of flapper mechanism with piezo actuator is characterized using Bouc-Wen model and displacements of flapper is controlled and monitored with both laser displacement sensor and strain gage and also control methods with voltage amplifier are tested in Bouc-Wen model hysteresis compensator, close loop with PI controller and hybrid control in test setup. The hysteresis errors are compared with each others.

## Biography

Ihsan Burak Temelturk has received his BS degree in Mechanical Engineering in 2012 and completed Master of Science degree from Aerospace Engineering Department in Middle East Technical University in Ankara, Turkey. He is currently a System Design Engineer in Turkey. His research interests include design, modeling and control of electromechanical systems. He has studied piezo materials, piezo actuators and its applications.

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**Notes:**

Igor Y Denisyuk et al., J Material Sci Eng 2017, 6:2 (Suppl)
http://dx.doi.org/10.4172/2169-0022.C1.061

# Nano-biocomposites for biomedical application

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Silver, gold, selenium and metal oxides nanoparticles in polymer matrix intensively investigated in biomedical application due to the plenty of unique properties of antimicrobial properties to Gram-positive, Gram-negative pathogens and antifungal activity is an important scientific problem to create bio-nanocomposites. Non-selective, broad spectrum antibacterial and antifungal activity against different types of microorganisms as well as the long-term effect for a few months is one of the main requirements to biopolymers. Nanocomposites with nanoparticles Ag, Au, $SiO_2$, ZnO were prepared on the basis of two monomer compositions: (1) Acidic composition consisting of monomers: 2-Carboxyethyl and Bisphenol A glycerolate. (2) pH neutral formulation consisting of monomers: Diurethanedimethacrylate and Isodecyl acrylate and photo initiator. Methods of preparing polymer films based nanocomposites can be found in our papers. Exposure was increased 5 times from total time of polymerization for these composites; prepared samples were heated at 50°C for 12 hours to minimize the effects of residual monomers in the experiment. As test objects were used: Strains of fungi *Candida albicans (C. albicans* NCTC 885-653) and *Aspergillus fumigatus* (clinical isolate); strains of staphylococci Community-associated Methicillin-resistant *Staphylococcus aureus* (CA-MRSA, penicillin-binding protein (PBP2α) - positive); Healthcare-associated Methicillin-resistant *Staphylococcus aureus* (HA-MRSA, penicillin-binding protein (PBP2α) - positive); Methicillin-resistant *Staphylococcus epidermidis* (MRSE, penicillin-binding protein (PBP2α) - positive); Methicillin-resistant *Staphylococcus epidermidis* (MRSE, penicillin-binding protein (PBP2α) - negative); Methicillin-resistant *Staphylococcus aureus* (MRSA, penicillin-binding protein (PBP2α) -negative); Methicillin-susceptible *Staphylococcus aureus* (MSSA); Methicillin-susceptible *Staphylococcus epidermidis* (MSSE). The antifungal activity of ZnO nanocomposites based on polymeric matrix 2-Carboxyethyl acrylate/Bisphenol-A-glycerolate (1 glycerol/phenol) diacrylate against *C. albicans* and *A. fumigatus* was found. Pronounced suppressive effect of ZnO nanocomposites based on polymeric matrix 2-Carboxyethyl acrylate/Bisphenol-A-glycerolate (1 glycerol/phenol) diacrylate against staphylococci was identified. The antifungal activity of polymeric matrix based on 2-Carboxyethyl acrylate/Bisphenol-A-glycerolate (1 glycerol/phenol) diacrylate against *C. albicans* was found.

## Biography

Igor Y Denisyuk has his expertise in field of nanoparticles, non-linear molecular crystals, polymer material, photonics, phodegradable nanocomposites and biomedical nanocomposites.

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## Notes:

Masahide Terazima, J Material Sci Eng 2017, 6:2 (Suppl)
http://dx.doi.org/10.4172/2169-0022.C1.061

# Advanced light sensing natural proteins that can detect light intensity

**Masahide Terazima**
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There are many photo-response biological proteins to convert the light energy to chemical energy, or to generate light information. It may be possible to use these proteins as advanced materials to detect light. For such applications, it is necessary to understand the molecular mechanism of the light detection of these proteins. In general, revealing conformation changes and intermolecular interactions is essential for the understanding. Although optical spectroscopies developed so far have been used for detecting dynamics of chemical reactions, there are many undetectable (spectrally silent) dynamics in biological reaction systems by these methods. It is desirable to develop a method to overcome this limitation. We have succeeded in detecting many intermediate species, which cannot be detected by traditional spectroscopic methods. The principle is based on the time-resolved detection of energies, volume changes, and the diffusion coefficient changes by the time-resolved transient grating (TG) method. Here I will demonstrate the method on a reaction of a blue-light sensor protein: PixD. We found a very unique light intensity dependence of the reaction, which may be used as an advanced material for the light sensor. PixD proteins are ones of photosensors containing the BLUF domain. They include Slr1694 (SyPixD) and Tll0078 (TePixD). SyPixD regulates phototaxis of cyanobacterium. Crystallographic analyses showed that these homologous PixD proteins have oligomeric structures: a decamer comprised of two stacked pentameric rings. We found that the dissociation reaction of the decamer is a key reaction for signal transduction and it will be used for application purpose. By using the TG technique, we discovered that the conformational change of the TePixD and SyPixDdecamer depend on the intensity of the excitation light. From the excitation light intensity dependence, we found that the multiphoton excitation of this protein is essential for the reaction.

## Biography

Masahide Terazima has his expertise in physical chemistry for elucidating reaction mechanism. In particular, his current research interests are studies of chemical reaction dynamics of biological proteins. He has been developing new methods for direct detection of energy and conformation of reactive species in time-domain. Furthermore, he has succeeded in measurement of molecular diffusion processes in time-domain. He has discovered that the diffusion coefficient is sensitive to protein conformations, so that this technique can be used for tracing dynamical conformation change as well as intermolecular interaction changes.

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**Notes:**

Nathan P Salowitz et al., J Material Sci Eng 2017, 6:2 (Suppl)
http://dx.doi.org/10.4172/2169-0022.C1.061

## Mechanics based design and testing of crack closing self-healing materials to carry external loads

**Nathan P Salowitz, Ameralys Correa, Afsaneh Moghadam** and **Pradeep Rohatgi**
University of Wisconsin-Milwaukee, USA

Self-healing materials have innate capabilities to restore geometry and mend damage in a structure. These materials have tremendous potential to prevent catastrophic failures and overcome fatigue issues by repairing structural damage as it occurs, while in service. In order to restore bulk deformations and close macroscopic cracks self-healing materials have been developed that are essentially sparse fiber composites, composed of a structural matrix reinforced with shape memory fibers. This composition is capable of closing large cracks and restoring bulk geometry in a free, unloaded state. A significant limitation of this technique is that structures are not capable of overcoming or withstanding externally applied loads while restoring their original geometry. This is because the shape memory material used to restore geometry is currently cast in its trained geometry. Therefore, activation and recovery will only provide loads to return to that original geometry, negating plastic deformation of the matrix and any externally applied load will cause deviation, inhibiting geometric restoration. Seeking to overcome this limitation, polymer samples were created containing prestrained nickel titanium shape memory fibers that undergo constrained recovery upon activation. Actuation of the shape memory fibers generates internal/residual loads allowing the healed structure to withstand and overcome externally applied loads. Theory, experimental results, analysis and future vision for self-healing materials composed of prestrained nickel titanium shape memory fibers are discussed. A mechanics based derivation is presented relating internal/residual loads to allowable externally applied loads. Experimental results are presented from samples composed of prestrained shape memory alloy reinforced polymer with an internal framework to ensure load transfer between components. Samples were loaded in tension with a constant crosshead speed until matrix failure, then healed through thermal actuation and loaded to crack opening multiple times. Analysis of theory and experimental results are presented.

### Biography

Nathan P Salowitz has received his BS degree in Engineering Mechanics from the University of Wisconsin Madison in 2001 and MS and PhD degrees in Aeronautics and Astronautics from Stanford University in 2006 and 2013, respectively. From 2003 to 2005, he was a Structural Analysis Engineer with The Boeing Company. From 2013 to 2014, he was a Postdoctoral Engineering Research Associate at Stanford University. Since 2014, he has been an Assistant Professor with the Mechanical Engineering Department with Adjunct Professor Appointments in the Electrical Engineering and Civil and Environmental Engineering departments at the University of Wisconsin-Milwaukee. He has more than 16 publications and is currently pursuing research in intelligent materials and structural health monitoring with particular interests in sensor design, mass sensor deployment, wireless communication and the interaction of sensors and structures.

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**Notes:**

An-Yi Chang et al., J Material Sci Eng 2017, 6:2 (Suppl)
http://dx.doi.org/10.4172/2169-0022.C1.061

# Microfluidic-enabled electrochemical studies of boron-doped ultrananocrystalline diamond microelectrodes for chronic neurochemical sensing

**An-Yi Chang, Gaurab Dutta** and **Prabhu U Arumugam**
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Electrochemical microsensors play an important role in investigating the effect of neurochemicals in human brain function. Abnormal levels of neurochemicals cause several neurodegenerative diseases. The current microelectrodes foul rapidly in brain microenvironment and results in significant reduction in chemical sensitivity and sensor's useful lifetime. Here, we present boron-doped ultrananocrystalline diamond (BDUNCD) microelectrodes that could aid in long-term monitoring of neurochemicals because of their wide electrochemical potential window, extremely low background current and excellent chemical inertness. The research goal is to reduce the rate of electrode fouling arising from reaction byproducts (e.g., melanin) and extend the lifetime to several weeks, which does not exist now. We microfabricated a custom microfluidic platform to study the BDUNCD surface fouling mechanism by depositing and mapping silver particles on BDUNCD microelectrode surfaces that were fouled at different conditions. The rate of fouling was studied using Fast Scan Cyclic Voltammetry (FSCV) and Amperometry (AM) techniques. For the first time, in situ electrode cleaning methods were developed to extend the electrode lifetime by >4-fold. Finally, chemical sensitivity enhancements were investigated by modifying BDUNCD with carbon nanotubes (CNT) and polymer coatings. For this study, we developed a droplet microfluidic device to study the changes in sensitivity and response time to two neurochemicals (dopamine and serotonin) using three different microelectrode surfaces.

## Biography

An-Yi Chang is currently pursuing his PhD with his major in Micro- and Nanoscale Systems at Louisiana Tech University, USA. He has earned his MS in Chemical Engineering from Louisiana Tech University, USA. His research emphasis on biological microfluidics, particularly, designing microfluidics to study cell reactions and drug release in microenvironments. Presently, he is working in Institute for Micromanufacturing (IFM) and concentrating on developing microfluidics for on-chip biosensing of neurochemical sensing with boron-doped nanocrystalline diamond microelectrodes (BDUNCD).

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**Notes:**

Peng-Sheng Wei, J Material Sci Eng 2017, 6:2 (Suppl)
http://dx.doi.org/10.4172/2169-0022.C1.061

# Mechanisms of mass transfer on porosity during solidification

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Pore formation and its shape in solid influence not only microstructure of materials, but also contemporary issues of various sciences of biology, engineering, foods, geophysics and climate change, etc. In order to remove and control porosity, understanding its formation is important. A pore formed in solid is a consequence of a bubble nucleated by super-saturation and entrapped by a solidification front. This work accounts for realistic mass and momentum transport across a self-consistently and analytically determined shape of the bubble cap, whose surface is in physico-chemical equilibrium beyond the solidification front. Accurate determination of contact angle from a realistic shape of the cap is required to predict the relevant shape of the pore in solid. It was systematically found that there are two different solute transport models subject to thin and thick thicknesses of concentration boundary layers on the solidification front. Case 1 accounts for species transport from the pore across an emerged cap through a thin concentration boundary layer on the solidification front into surrounding liquid in the early stage, whereas Case 2 is subject to species transport from the surrounding liquid across a submerged cap within a thick concentration boundary layer into the pore. The analytical results find that the variation of solute gas pressure in the pore with time determines development of the pore shape in solid. Increases in mass transfer coefficient and solidification rate decrease the pore radius. The predicted pore shape agrees with experimental data. A realistic prediction and control of the growth of the pore shape has therefore been obtained.

## Biography

Dr. Peng-Sheng Wei received Ph.D. in Mechanical Engineering Department at University of California, Davis, in 1984. He has been a professor in the Department of Mechanical and Electro-Mechanical Engineering of National Sun Yat-Sen University, Kaohsiung, Taiwan, since 1989. Dr. Wei has contributed to advancing the understanding of and to the applications of electron and laser beam, plasma, and resistance welding through theoretical analyses coupled with verification experiments. Investigations also include studies of their thermal and fluid flow processes, and formations of the defects such as humping, rippling, spiking and porosity. Dr. Wei has published more than 80 journal papers, given keynote or invited speeches in international conferences more than 90 times. He is a Fellow of AWS (2007), and a Fellow of ASME (2000). He also received the Outstanding Research Achievement Awards from both the National Science Council (2004), and NSYSU (1991, 2001, 2004), the Outstanding Scholar Research Project Winner Award from National Science Council (2008), the Adams Memorial Membership Award from AWS (2008), the Warren F. Savage Memorial Award from AWS (2012), and the William Irrgang Memorial Award from AWS (2014). He has been the Xi- Wan Chair Professor of NSYSU since 2009, and Invited Distinguished Professor in the Beijing University of Technology, China, during 2015-2017.

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**Notes:**

3rd International Conference on

# Smart Materials & Structures

March 20-22, 2017 Orlando, USA

# Scientific Tracks & Abstracts

## Day 2

Kirk J Ziegler et al., J Material Sci Eng 2017, 6:2 (Suppl)
http://dx.doi.org/10.4172/2169-0022.C1.061

# Modulating the surfactant structure around single wall carbon nanotubes for single chirality separations

**Kirk J Ziegler, Yang Zhao** and **Jia Xu**
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The post synthesis separation of single wall carbon nanotubes (SWCNTs) is needed for their inclusion in novel electronic devices. For example, semiconducting SWCNTs have unique optoelectronic properties that can be utilized in photovoltaics and biosensors. The high surface area of nanomaterials dictates that the interface with their surroundings is important in determining their properties or functionality. For example, all atoms in SWCNTs exist on the surface and therefore, have excellent sensing capabilities. The interface of SWCNTs with their surroundings is also important to their application in polymer composites, devices, drug delivery, bioimaging and biosensing. SWCNT interfaces are often altered with surfactants to improve their dispersion in aqueous suspensions. Understanding and ultimately controlling these surface layers is important because of its influence on reactivity, adsorption of pollutants and interaction with materials. Our group has focused on characterizing and controlling SWCNT interfaces for high-fidelity separations of semiconducting SWCNTs by the n, m type. Here we report the high-fidelity desorption of single-chirality SWCNTs from hydrogels through surfactant structure modulation. High-purity fractions of (n, m) SWCNTs are obtained with high yield once a specific ratio of sodium dodecyl sulfate (SDS)/sodium deoxycholate (DOC) co-surfactant solution is used as the eluent. The elution of only one n, m type at a specific co-surfactant ratio while other types are exposed to more surfactant suggests that each n, m type forms a thermodynamically-stable surfactant structure in the co-surfactant solution.

## Biography

Kirk J Ziegler has joined the Chemical Engineering Department at the University of Florida in 2005. His work on SWCNTs has focused on understanding the effect of surfactant-nanotube interactions on dispersion and separation processes. His work on nanowire arrays has applications in energy-related devices, which require high surface area to maximize energy generation or storage.

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## Notes:

Avinash Baji et al., J Material Sci Eng 2017, 6:2 (Suppl)
http://dx.doi.org/10.4172/2169-0022.C1.061

# Fabrication of hierarchical structures using electrospinning for dry adhesive applications

**Avinash Baji** and **Rahul Sahay**
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In this study, hierarchical structures for dry-adhesive applications were fabricated using electrospinning combined with template wetting method. Briefly, in the first step, electrospinning technique was used to produce micron sized fibers which were directly deposited on porous anodized aluminum oxide (AAO) template. Following this step, the setup consisting of the AAO template along with the fibers was heated above the glass transition temperature of polymer. This enabled the flow of polymer within the porous channels and resulted in the growth of nanometer sized pillars on the surface of the fibers. Based on this fabrication technique, we produced hierarchical structures using two different polymeric systems, viz. poly(methyl methacrylate) (PMMA) and poly(vinylidene fluoride) (PVDF). A representative scanning electron microscopy (SEM) image of the fibers is shown in Figure-1. The SEM image shows that this approach led to the growth of sub-nano structures on the surface of the fibers. These samples were used to investigate the normal as well as shear adhesion behavior of hierarchical structures. The normal adhesion was characterized using a nanoindenter. A flat circular indenter tip (diameter=10 μm) was used to indent the surface of the samples and then retracted back. The pull-off required to separate the indenter tip from the samples was recorded. This pull-off force gave an indication of its normal adhesion. Similarly, the samples were finger pressed onto sandpaper with varying degree of roughness. The samples were then pulled in shear and the shear adhesion force was characterized. Fibers without any surface structures were also tested and their adhesion behavior was compared with that of hierarchical samples. The samples with surface nanostructures exhibited increased pull-off force compared to neat control samples due to its improved van der Waals interactions.

## Biography

Avinash Baji focuses on bio-inspired materials research using electrospun polymer fibers. His current research interests include fabrication of electrospun fibers for dry adhesion applications. He aims to mimic the geometry and adhesive mechanisms of natural materials using electrospinning enabled techniques. He has authored over 35 journal articles with additional papers in conference proceedings.

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## Notes:

Adel Najar et al., J Material Sci Eng 2017, 6:2 (Suppl)
http://dx.doi.org/10.4172/2169-0022.C1.061

# Enhanced surface passivation effect in porous GaN for high performance $H_2$ gas sensors at room temperature

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Diatomic hydrogen is a colorless, odorless, and tasteless gas which, when combined with air, poses a safety hazard due to its wide flammability range where high burning velocities and explosive tendencies compound the risks. At high concentrations it can also act as an asphyxiant. Its importance stems primarily from its use as a reactant for the chemical industry in the processing of ammonia, petrochemicals, and methanol. Effective $H_2$ sensors that can quickly and sensitively respond to $H_2$ gas are crucial for the safe deployment of all hydrogen-based applications. Ideally, a $H_2$ gas sensor should be compact, sensitive, and durable, have short response times, and be simple to fabricate. We describe the fabrication of porous GaN prepared by metal electroless etching method. Then, porous GaN was treated by octadecylthiol (ODT) for the passivation of the surface states. At room temperature, the passivation of the porous GaN sample enhance the detection of $H_2$ gas. After passivation using ODT, the sample show excellent selectivity compared to other gases (i.e. $H_2S$, $C_2H_4$). Simultaneously, this sensors exhibited good sensing repeatability and stability. This enhancement in gas sensing properties after passivation was attributed to the effect of ODT to reduce the surface states effect. The attractive low-cost, low power consumption and high performance of the resultant passivation porous GaN gas sensor assure their potential application for $H_2$ gas sensor working at low temperature.

## Biography

Adel Najar received his PhD in Physics at ENSSAT- Rennes 1 University in France and MBA from Beuth Hochschule Fur Technik Berlin in Germany in 2007 and 2016, respectively. He served as a post-doctorat at Saint-Gobain Research Company in collaboration with Grenoble Institute of Technology in France, a Research Scientist at LETI at the Alternative Energies and Atomic Energy Commission (CEA) in France as well as at KAUST in Saudi Arabia, and Senior Research Scientist at Atsugi R&D Center, NTT Corp. in Japan. From 2015, Dr. Najar appointed as faculty in UAE University in UAE. His main research interests is the development of semiconductor nano-structure for photonics and nanophotonics application. Dr. Najar is an author and co-author of more than 50 papers in peer-reviewed journals, conferences, book chapter and patents.

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## Notes:

Neeru Chaudhary et al., J Material Sci Eng 2017, 6:2 (Suppl)
http://dx.doi.org/10.4172/2169-0022.C1.061

# Electrical resistivity change of SeTeAg compositions to thermal and pressure as stress

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To understand the behavior of materials for applications in solid state electronic devices, the materials are to be exposed to different stresses such as thermal, electrical, humidity, optical, nuclear radiations, pressure (static or dynamic) etc. to better understand their structural, morphology, conduction, optical and sensing properties. The $Se_{85}$-$xTe_{15}Ag_x$ compositions prepared from melt-quench technique were exposed to High Pressure (0-10 GPa) and Temperature (300K-373K). The results depict the change in resistivity with respect to pressure in forward as well as backward pressurization. These results depicts that there is very small change in resistivity with change in pressure and the change in resistivity with respect to pressure follows the same pattern, when the pressure is applied from atmospheric pressure to 10 GPa and vice versa. The results of resistivity change with the variation of Silver in the compositions are also reported in this study. Similar results are observed in case of resistivity change with respect to temperature. Some deviation is observed in the results which are well explained with average coordination number, fermi level change and crystallinity.

## Biography

Er. Neeru Chaudhary is an Assistant Professor in Department of Physics, Panjab University, Chandigarh. She got her B.E. in Instrumentation in 1999 from Dr. B.A.M. University, Aurangabad (M.S.) and M.Tech in Instrumentation from University Centre of Instrumentation and Microelectronics, Panjab University Chandigarh in 2001. Currently Er. Neeru Chaudhary's research is focused on studying Electrical and Optical properties of Semiconductor materials to be used in solid state electronic devices. The rapid growth in the field of MEMS and NEMS has led to production of variety of new materials. Hence the study of properties of the materials under different stresses is very important field in Material Science Engineering. She is life member of two national professional bodies; Indian Society of Technical Education (ISTE) and Indian Association of Physics Teachers (IAPT).

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**Notes:**

Naser Qamhieh et al., J Material Sci Eng 2017, 6:2 (Suppl)
http://dx.doi.org/10.4172/2169-0022.C1.061

# Optical and electrical characterization of Co doped Ge-Sb-S films

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Thin films of amorphous Germanium antimony sulfide (Ge30Sb10S60) doped with cobalt (Co) have been deposited on glass substrates by thermal evaporation technique. The composition and amorphous structure of the deposited films have been characterized by X-ray diffraction and energy dispersive X-ray analysis (EDX) techniques. Optical transmission spectra measured by UV-VIS spectrophotometer showed that Co-doped Ge30Sb10S60 have 2.0 eV optical band gap. Raman spectroscopy was used to characterize the composition and phase structure of the prepared film and shows a wide band spectrum from 300 to 410 cm$^{-1}$ centered at 355 cm$^{-1}$. The Raman shift peaks at 325 cm$^{-1}$ and 350 cm$^{-1}$ are assigned to the bond stretching mode Sb-S and Ge-S, respectively. The capacitance and conductance versus voltage measurements were performed at different temperatures. The results show a slight increase in the capacitance with temperature and it reaches a maximum value around 150$^{o}$C and eventually it becomes negative. This behavior is interpreted in terms of the nucleation-growth process and the thermally activated conduction process with measured activation energy of 0.79 eV. This value of activation energy together with the measured optical gap indicates that the Fermi level is unpinned in the gap which could be attributed to gap states induced by cobalt doping.

## Biography

Naser Qamhieh has received his PhD in Physics in 1996 from the University of Leuven, Belgium, where he worked with professor Guy Adriaenssens. He has joined the Department of Physics at United Arab Emirates University (UAEU) in 1999 where he is presently a full Professor. His research interest centers on experimental study of the electronic properties and density of states of amorphous semiconductors and chalcogenide glasses and among materials of interest is phase change materials used in memory devices. His research also involves fabrication and characterization thin films and nanoclusters by the existing techniques in UAEU labs. He has published over 50 research articles in refereed international journals and conferences. He was honored a Research Project Award by the Research Affairs at UAE University in 2009. Moreover, he has rich experience in teaching and developing general physics courses in UAEU. He had several contributions to pedagogical journals and conferences. For research in pedagogy, he was honored the 2009-2010 Faculty of Science Recognition Award for Excellence in Teaching and Learning.

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Michael N Leuenberger et al., J Material Sci Eng 2017, 6:2 (Suppl)
http://dx.doi.org/10.4172/2169-0022.C1.061

# Electronic and optical properties of transition metal dichalcogenides in the presence of vacancy defects

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Single layer (SL) transition metal dichalcogenides (TMDCs) ($MX_2$; M=transition metal such as Mo, W and X= S, Se, Te) have attracted a lot of attention due to their intriguing electronic and optical properties. SL TMDCs are direct band gap semiconductors, which can be used to produce smaller and more energy efficient devices such as transistors and integrated circuits. Moreover, the band gap lie in the visible region, which makes them highly responsive when exposed to visible light, a property with potential applications in optical detection. In contrast to graphene, SL TMDCs exhibit large spin-orbit coupling (SOC) originating from the d orbitals of the transition metal atoms. The presence of the giant SOC makes them great candidates for exploring spin physics and for spintronic devices. Defects usually play an important role in tailoring electronic, optical and magnetic properties of semiconductors. We performed standard first-principle study to evaluate the electronic and optical properties of single-layer (SL) transition metal dichalcogenides (TMDCs), in the presence of vacancy defects (VDs). We consider three types of VDs in SL TMDCs (1) X-vacancy, (2) $X_2$-vacancy, and (3) M-vacancy. We find that VDs lead to localized defect states (LDS) in the band structure, which in turn give rise to sharp transitions in in-plane and out-of-plane optical susceptibilities, $\chi\Pi$ and $\chi\perp$, respectively. The effects of spin orbit coupling (SOC) are also considered. We find that SOC splitting in LDS is directly related to the atomic number of the transition metal atoms. Apart from electronic and optical properties we also find magnetic signatures (local magnetic moment of $\sim\mu_B$) in $MoSe_2$ in the presence of Mo vacancy, which breaks the time reversal symmetry and therefore lifts the Kramers degeneracy. We use group theory to derive the optical selection rules for both $\chi\Pi$ and $\chi\perp$.

## Biography

Michael N Leuenberger has received his PhD degree in Theoretical Physics in 2002 from the University of Basel in Switzerland. After his Postdoctoral positions at the University of Iowa and at the University of California, San Diego he joined in 2005 the NanoScience Technology Center at the University of Central Florida and became tenured Associate Professor in 2011. In 2008, he has received the DARPA/MTO Young Investigator Award. His current research areas include quantum information processing in topological insulators, optoelectronics in 2D materials and solar energy harvesting in nanoparticles. He has published more than 60 peer-reviewed papers and 4 book chapters.

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**Notes:**

Pankaj Sharma et al., J Material Sci Eng 2017, 6:2 (Suppl)
http://dx.doi.org/10.4172/2169-0022.C1.061

# Fabrication of low resistive and stable Li-P co-doped *p*-type ZnO by dual ion beam sputtering

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In the last decade, Zinc oxide (ZnO) based optoelectronic devices have attracted much attention due to their superior material properties such as wide direct band gap energy, large exciton binding energy, high radiation resistance and chemical and thermal stability. However, the lack of availability of reliable and stable *p*-type ZnO has always remained a concern in order to fabricate these devices. Various groups have reported *p*-type ZnO by doping with different elements of group V, whereas others have also used co-doping approach for achieving *p*-type conduction in ZnO. Unfortunately, the high resistivity and low hole concentration still poses limitations for high performance devices. In this work, we report the fabrication of high hole concentration, low resistive and stable Li-P co-doped ZnO (LPZO) thin films. LPZO thin films were fabricated by DIBS technique on low resistive *n*-type Si substrates. The deposition was performed using high quality ceramic target having Li and P content of 5% and 3% respectively, in oxygen rich ambient at 300°C and 500°C. Post deposition annealing was carried out in N2 ambient at 800°C for 20 minutes to activate the acceptor dopants. The XRD pattern of annealed LPZO film confirmed that crystal structure was preferentially oriented in *c*-axis (002) direction. FWHM of (002) peak was calculated to be 0.24° resulting in a crystallite size of ~35 nm. It shows the schematic structure of *p*-LPZO/*n*-Si heterojunction with linear I-V curves of ohmic contacts. Hall measurement was performed in the van der Pauw configuration to measure the electrical parameters e.g., carrier concentration, resistivity and mobility. The annealed LPZO films clearly depicted *p*-type conduction as observed from the rectifying behavior. A relatively higher hole concentration of the order $2\times10^{20}$ cm$^{-3}$ and resistivity of $8\times10^{-3}$ Ω.cm were calculated. The turn-on voltage of the diode was determined to be 1.6 V whereas the rectification ratio of forward to reverse current at ±3 V was 76.

## Biography

Pankaj Sharma is currently pursuing his PhD degree in Electrical Engineering at Indian Institute of Technology Indore since 2014. He has completed his Masters in VLSI Design from Delhi, India. His research work includes fabrication and characterization of ZnO thin films using dual ion beam sputtering technique for optoelectronic applications. He is presently working on realizing low resistive and high hole concentration ZnO thin films by using various acceptor dopants.

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## Notes:

3rd International Conference on

# Smart Materials & Structures

March 20-22, 2017 Orlando, USA

# Scientific Tracks & Abstracts

## Day 3

Satilmis Basan et al., J Material Sci Eng 2017, 6:2 (Suppl)
http://dx.doi.org/10.4172/2169-0022.C1.061

# Thermal degradation of two tung oil based reactive diluents and linseed oil alkyd

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Thermal degradation of two tung oil based reactive diluents, linseed oil alkyd and different amounts of two reactive diluents having paint formulations were investigated using TGA and DSC under non-isothermal conditions and dynamic nitrogen atmosphere and air. Activation energies were obtained from Freidman method and Freeman-Carroll method and subsequently the pre-exponential factor 'A' and reaction order 'n' for reactive diluents and alkyd were also determined according to general rate equation. From kinetic analysis of the thermal degradation of using TGA, it was founded that thermal degradation of two diluents and alkyd has taken place in one stage but thermal degradation of all paint formulations have taken place in more than two stages. As shown from Freidman method and Freeman-Carroll method, the chemical composition and atmosphere of reactive diluents influenced the thermal degradation. Increasing reactive diluents decreased slightly the thermal stability of linseed oil alkyd.

## Biography

Satilmis Basan has completed his PhD from Hacettepe University and Postdoctoral studies from Glasgow University, Department of Chemistry and Akron University, Department of Polymer Engineering. He is the Head of Department of Chemical Engineering, Founder Dean of Faculty of Engineering at Hittite University and Editor in Chief of Journal of the Turkish Chemical Society, Section B: Chemical Engineering. He has published more than 24 papers in reputed journals.

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## Notes:

Ioana Csaki et al., J Material Sci Eng 2017, 6:2 (Suppl)
http://dx.doi.org/10.4172/2169-0022.C1.061

## In situ geothermal test results for multilayer coated steel

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Geothermal steam contains dissolved minerals that can precipitate from the liquid and deposit onto the surface of the blades and rotors used for turbine producing geothermal energy. This process is called scaling and it occurs due to a change in temperature, pressures or pH values of the geothermal fluid disturbing the equilibrium of the system. When scaling occurs in geothermal equipment can create major problems in geothermal power production. A solution to avoid these problems consists in coating the steel made turbine blade with different materials layer. These coatings will provide corrosion and erosion resistance and durability for the equipment used in geothermal energy. Samples coated with Ni base alloy and Y using high velocity oxygen fuel technique was investigated after in situ testing in Hellisheiði power plant in Iceland. This paper aims to investigate the microstructure, physical and chemical properties of the coating providing a view on the composite materials behavior under geothermal steam. The studied composite powders are designed to prevent corrosion damages and have good reliability during the geothermal turbines life. Powder multi-component and composite layers obtained were investigated using a system characterization by X-ray difractometer and SEM and EDX analysis to obtain detailed information about the complex modifications inside of the structure and on interface deposition.

### Biography

Ioana CSAKI, Associate professor, is working in Engineering and Management of Metallic Materials Production Department, Materials Science and Engineering, University Politehnica Bucharest, She published a series of 5 books, and over 45 articles and conference papers from which: 16 articles in ISI journals and proceedings and 32 articles in journals indexed in international data base. She was project partner for 3 international research grants, 1 being the project manager on behalf of UPB and participation at over 48 research national grants. She is also project manager for EEA grants collaboration between University Polytechnic Bucharest and University of Iceland. The research directions approached were metallic powders processing for new multi-component materials through powder metallurgy advanced materials, composite materials, high entropy alloys with very good mechanical properties and multi-component materials for coating parts submitted to high corrosion environment and high wear.

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**Notes:**

Wolfgang Sigmund, J Material Sci Eng 2017, 6:2 (Suppl)
http://dx.doi.org/10.4172/2169-0022.C1.061

## Smart nanomaterials structures

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Surfaces are key for applications that require sticking or non-sticking, high or low friction. We recently investigated surfaces of plants and spiders and transferred these findings into synthetic surfaces. This talk will present three foci: Plastron surfaces that repel all liquids, repulsive van der Waals surfaces for quantum lubrication and tunable surfaces that respond in microseconds to stimuli. By mimicking surface structures of spiders we are able to reduce contact of water and sticking of water droplets to surfaces yielding perfectly spherical droplets without the need for fluorinated compounds. Modifications of these hairy nanostructures are capable of also repelling low surface tension liquids and oils. To further the non-sticking behavior we also investigate quantum mechanical non-sticking surfaces. By tailoring the electronic properties of engineered surfaces we can achieve repulsive van der Waals forces which are the first step towards permanent quantum lubrication. The last part of the talk will discuss how nanofibers in other morphologies can be produced and used to make surfaces that can respond within microseconds to environmental stimuli. Thus a rotating tire can be designed that may respond to the road condition (temperature or moisture) the moment it touches the road and adjust its adhesion according to its design.

### Biography

Dr. Sigmund is currently Professor of Department of Materials Science and Engineering at University of Florida, USA. He obtained a B.S. in Chemistry from the University of Heidelberg, Germany. Before obtaining his Ph.D. at the Gutenberg-University of Mainz, he began work on colloidal particle systems at the Max-Planck-Institute for Polymer Research in Mainz with Prof. G. Wegner. In the early 1990's, Dr. Sigmund held post-doctoral positions. He was at RIKEN's (located in Japan) Frontiers of Nanoscience Program in 1992. Then he joined the Max-Planck Institute of Metals research and moved to the University of Florida in 1999. His main focus is on the interdisciplinary development, synthesis, and characterization of novel materials such as nanomaterials for energy harvesting and storage; colloid and surface science; fusion of bioenergy systems with engineered systems; electrospinning of nanomaterials; enhancing materials' properties.

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**Notes:**

Hussein Alrobei et al., J Material Sci Eng 2017, 6:2 (Suppl)
http://dx.doi.org/10.4172/2169-0022.C1.061

# α-hematite-molybdenum disulfide and polyhexylthiophene (RRPHTh)-nanodiamond (ND) electrodes for photoelectrochemical applications

**Hussein Alrobei** and **Manoj K Ram**
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The alpha (α)-hematite ($Fe_2O_3$) nanomaterial is attractive due to its band gap, chemical robustness, availability in the nature and excellent photoelectrochemical (PEC) properties to split water into oxygen and hydrogen. However, the α-$Fe_2O_3$ suffers from low conductivity, slow surface kinetic, low carrier diffusion and greater electron-hole combination. The electronic properties such as carrier mobility and diffusion of α-$Fe_2O_3$ can be improved through doping, synthesis of composite material or formation of structured films. Recently, 2D-molybdenum disulfide ($M_oS_2$) has shown interesting photocatalytic activity due to its bonding, chemical composition, doping and nanoparticles grown on other 2D-film. Recently, our group has studied photoelectrochemical properties of hybrid film of regioregular poly (3-hexylthiophene-2, 5-diyl) (P3HT) with nanodiamond as well as P3HT-$M_oS_2$. In the present study, we have studied photoelectrochemical properties of polyhexylthiophene (RRPHTh)-nanodiamond (ND) and α-$Fe_2O_3$-$M_oS_2$ nanocomposite based electrodes films. The photoelectrochemical properties of α-$Fe_2O_3$-$M_oS_2$ as n-type and ND-RRPHTh as p-type electrodes in photoelectrochemical cell in various electrodes have been studied. We have obtained 3 to 4 times higher photocurrent and energy conversion efficiencies than the parent electrode based photoelectrochemical cell. We have synthesized nanocomposite α-$Fe_2O_3$-$M_oS_2$ using sol-gel technique. The nanocomposite α-$Fe_2O_3$-$M_oS_2$ as well as ND-RRPHTh films were characterized using SEM, X-ray diffraction, UV-vis, FTIR and Raman techniques. The electrochemical techniques were used to understand the photocurrent in electrode/electrolyte interface of α-$Fe_2O_3$-$M_oS_2$ as well as ND-RRPHTh films in both acid base based electrolyte. The α-$Fe_2O_3$-$M_oS_2$ and ND-RRPHTh electrodes reveal improved production of hydrogen compared to α-$Fe_2O_3$ and aluminum doped α-$Fe_2O_3$ and $M_oS_2$ doped α-$Fe_2O_3$ nanostructured films. The band structure has been used to understand the mechanism of photoelectrochemical water splitting in p-n types based photoelectrochemical cell.

## Biography

Hussein Saad Alrobei is a PhD candidate at Mechanical Engineering Department,University of South Florida, USA and lecturer at Mechanical Engineering Department, Prince Sattam Bin Abdulaziz University, Saudi Arabia.

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## Notes:

Dimitar Dimov, J Material Sci Eng 2017, 6:2 (Suppl)
http://dx.doi.org/10.4172/2169-0022.C1.061

## Graphene Reinforced Concrete

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The constant need for improvement of strength, ductility and durability of concrete is driving current research efforts towards improving the overall strength of concrete by nano-engineering its chemical and mechanical properties through reinforcement with nanomaterials. Graphene, an atomically thin layer of carbon, has a large specific surface area, high Young's modulus, high thermal conductivity and excellent electrical conductivity. These properties make graphene one of the most prominent nanomaterial for applications in concrete reinforcement.

Methodology: We report a novel method of increasing the overall compressive strength of concrete with the addition of defect-free, water-stabilised graphene dispersions. We demonstrate that the high-shear exfoliation of graphene in water is extremely efficient for the fabrication of graphene reinforced concrete as it can substitute water directly in the concrete mixture and it is industrially scalable.

Findings: Through a comparative statistical study of the mechanical properties of graphene reinforced and standard concrete we demonstrate that graphene reinforcement increases the strength of early age concrete by up to 18.6 %. Furthermore, our results show that the incorporation of graphene into the concrete matrix increases the compressive strength of the fully cured concrete by 26.

Conclusion & Significance: Our results indicate that the increase in early age compressive strength can contribute towards the urbanisation demands of constructing taller buildings by reducing the required time for keeping the formworks on construction sites, as well as by excluding the addition of chemical admixtures. A unique benefit is that unlike other nanomaterials, our method of production and final product are non-hazardous, making graphene reinforced concrete a promising material for a more environmentally friendly construction industry.

### Biography

Dimitar Dimov is a PhD researcher in Nanoscience and Civil Engineering at the University of Exeter, UK. Dimov has completed his BEng in Civil Engineering at Exeter and then was invited straight away to pursue a PhD degree after receiving the award for best individual research project (83%) during his final year of undergraduate. His current work bridges the international research on two-dimensional materials with traditional composite structural materials like concrete. The primary focus is to investigate the chemical and physical alterations of the cement hydration crystals upon the addition of nanomaterials.

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**Notes:**